REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
		FINAL

4. TITLE AND SUBTITLE

Theoretical Investigation of Superconductivity in Doped Fullerenes

5. FUNDING NUMBERS

61102F
2305/GS

6. AUTHOR(S)

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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

California Institute of Technology

8. PERFORMING ORGANIZATION REPORT NUMBER

AFOSR-TR- 95 0111

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFOSR/NE
110 Duncan Avenue Suite B115
Bolling AFB DC 20332-0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

F49620-92-J-0401

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

APPROVED FOR PUBLIC RELEASE: DISTRIBUTION UNLIMITED

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

SEE FINAL REPORT ABSTRACT

14. SUBJECT TERMS

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED

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FINAL TECHNICAL REPORT

F49620-92-J-0401

Project title: Theoretical Studies Relating to Superconductivity in Doped Fullerenes

Principal Investigator: Radi A. Jishi

The aim of the research we are conducting is to understand the phenomenon of superconductivity in the fullerene system. Towards achieving this goal we have conducted a series of studies and have published several papers quite recently.

1. We have developed a force-constant model for the C_{60} molecule which accounts for all measured frequencies in C_{60} [1]. The model employs four bond-stretching and four angle-bending force constants that were chosen to reproduce the correct values of the frequencies of the Raman-active vibrational modes. The model was successfully applied to higher fullerenes, such as C_{70}, and the effect of doping by alkali metal atoms on the phonon modes in C_{60} and in C_{70} was considered [2,3]. The study of the phonon spectrum in doped C_{60} and doped C_{70} is an important step in view of the fact that while doped C_{60} is superconducting, doped C_{70} is not. The studies we have carried out, combined with studies on the electronic states in doped C_{70}, could elucidate the difference in the electrical properties between these two materials.

We have considered the coupling of electrons to the intramolecular vibrational modes in C_{60} within the framework of the tight-binding model. The phonon eigenvectors were obtained from our force-constant model for C_{60}, and approximate electronic wave functions were used. We have found that, within the tight-binding model, it is possible to account for a transition temperature of approximately 30 K. Within this model, the high-frequency tangential modes couple more strongly to electrons than do the low-frequency radial modes. This is a direct consequence of the fact that while the tangential modes involve mainly bond-stretching displacements, the radial modes involve mainly angle-bending displacements. Nevertheless there is still some controversy concerning the phonon modes responsible for superconductivity; it is not yet firmly established that intramolecular vi-

brational modes play the crucial part. Actually, some NMR measurements are consistent with the proposition that doped C_{60} is a strong-coupling superconductor in which low-frequency intermolecular modes play an important role. Consequently, it is important to construct a model for the phonon dispersion in solid C_{60}, to calculate the phonon density of states, and to solve the Eliashberg equation for this system. This is currently under investigation.

2. A related problem, which is currently attracting a great deal of attention, is that of carbon nanotubes. These are produced either as multi-layered or single-layered systems. The fact that nanotubes may exhibit matallic or semiconducting properties, depending on their chirality, is of great importance. In particular, the possibility of superconducting behavior in single- or multi-layered tubes, or tubes filled with metallic atoms, such as Pb, is an intriguing proposition. We have investigated the symmetry properties of carbon nanotubes, and the consequences of these properties for the electronic states and the phonon modes in these tubes.[4,5] Furthermore, we have considered the electron-phonon coupling in single-layered metallic tubes and found that, under ideal conditions, their conductivity may exceed that of copper.[6] We are studying now, theoretically, the possibility of superconducting behavior in single- or multi-layered nanotubes.

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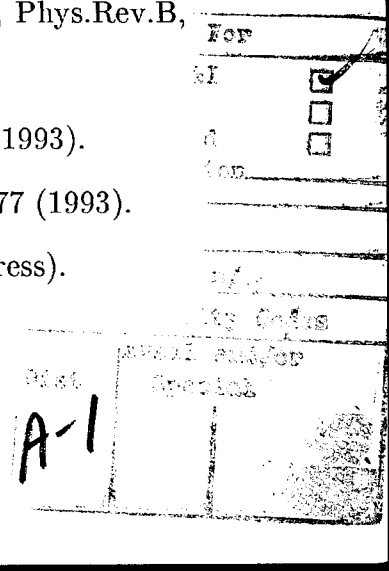

Technical Report
92-S-0401

Project: Theoretical Investigation of Superconductivity in Doped Fullerenes.
Principal Investigator: Radi A. Jishi

We have examined the strength of the electron-phonon coupling in alkali-metal doped C_{60} in order to determine the phonon modes that are primarily responsible for superconductivity in these materials. We started by calculating the wave functions of the molecular orbitals in C_{60} by diagonalizing a 60x60 matrix. The orbitals of interest for this problem are the 3-fold degenerate F_{1u} orbitals. The vibrational modes in C_{60} were calculated by a force constant model[1] that includes interactions up to the third nearest neighbors in order to determine accurately the phonon frequencies and eigenvectors for the H_g Raman-active modes, which are believed to be responsible for superconductivity in doped C_{60}. The electon-phonon coupling matrix elements are calculated within the tight binding approximation which works well for carbon systems. We have considered intra-band as well as inter-band electron-phonon scattering processes among the 3-fold degenerate F_{1u} bands.

We found that the inter-band coupling is as important as the intra-band coupling. The strength of the electron-phonon coupling for scattering between two different bands is approximately 60% of that within the same band. Out of the 8 H_g modes that are important for superconductivity, the coupling to electrons is

strong for four of them, namely, the $H_g(3)$, $H_g(5)$, $H_g(7)$, and $H_g(8)$, with frequencies given by 708 cm^{-1}, 1099 cm^{-1}, 1426 cm^{-1}, and 1575 cm^{-1}, respectively. The phonon mode most strongly coupled to electrons is $H_g(5)$, which alone accounts for 1/3 of the total coupling strength to electrons of all the modes together.

Another related problem we have recently dealt with is the electronic and vibrational states in carbon nanotubes and the coupling between them. [2,3] Although not realized yet experimentally, it is believed that one-dimensional channels exist in an array of nanotubes where dopant atoms can be incorporated. We will investigate the possibility of superconductivity in such systems in the near future. Starting from the electronic and vibrational states in a 2D graphene sheet, we have calculated, using the zone-folding method, the corresponding states in the nanotubes. Group theoretical techniques have been used in order to classify these states according to the irreducible representations of the relevant symmetry groups, thus setting the stage for investigating possible superconductivity in these systems.

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